

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:sssptal626gms

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America  
NEWS 2 Apr 08 "Ask CAS" for self-help around the clock  
NEWS 3 Apr 09 BEILSTEIN: Reload and Implementation of a New Subject Area  
NEWS 4 Apr 09 ZDB will be removed from STN  
NEWS 5 Apr 19 US Patent Applications available in IFICDB, IFIPAT, and IFIUDB  
NEWS 6 Apr 22 Records from IP.com available in CAPLUS, HCAPLUS, and ZCAPLUS  
NEWS 7 Apr 22 BIOSIS Gene Names now available in TOXCENTER  
NEWS 8 Apr 22 Federal Research in Progress (FEDRIP) now available  
NEWS 9 Jun 03 New e-mail delivery for search results now available  
NEWS 10 Jun 10 MEDLINE Reload  
NEWS 11 Jun 10 PCTFULL has been reloaded  
NEWS 12 Jul 02 FOREGE no longer contains STANDARDS file segment  
NEWS 13 Jul 22 USAN to be reloaded July 28, 2002;  
saved answer sets no longer valid  
NEWS 14 Jul 29 Enhanced polymer searching in REGISTRY  
NEWS 15 Jul 30 NETFIRST to be removed from STN  
NEWS 16 Aug 08 CANCERLIT reload  
NEWS 17 Aug 08 PHARMAMarketLetter(PHARMAML) - new on STN  
NEWS 18 Aug 08 NTIS has been reloaded and enhanced  
NEWS 19 Aug 09 JAPIO to be reloaded August 18, 2002

NEWS EXPRESS February 1 CURRENT WINDOWS VERSION IS V6.0d,  
CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP),  
AND CURRENT DISCOVER FILE IS DATED 05 FEBRUARY 2002  
NEWS HOURS STN Operating Hours Plus Help Desk Availability  
NEWS INTER General Internet Information  
NEWS LOGIN Welcome Banner and News Items  
NEWS PHONE Direct Dial and Telecommunication Network Access to STN  
NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 10:14:36 ON 13 AUG 2002

Golam Shameem

=> FIL REGISTRY  
COST IN U.S. DOLLARS

SINCE FILE ENTRY	TOTAL SESSION
0.21	0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 10:14:47 ON 13 AUG 2002  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
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STRUCTURE FILE UPDATES: 12 AUG 2002 HIGHEST RN 443729-39-3  
DICTIONARY FILE UPDATES: 12 AUG 2002 HIGHEST RN 443729-39-3

TSCA INFORMATION NOW CURRENT THROUGH January 7, 2002

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES  
for more information. See STNote 27, Searching Properties in the CAS  
Registry File, for complete details:  
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> s isoflavones?  
L1 0 ISOFLAVONES?

=> s isoflavones  
0 ISOFLAVONES  
L2 0 ISOFLAVONES

=> s flavones  
L3 1 FLAVONES

=> s flavone?  
L4 6194 FLAVONE?

=> FIL CAPLUS  
COST IN U.S. DOLLARS

SINCE FILE ENTRY	TOTAL SESSION
17.52	17.73

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 10:17:21 ON 13 AUG 2002  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
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of this information, without the prior written consent of CAS, is  
strictly prohibited.

FILE COVERS 1907 - 13 Aug 2002 VOL 137 ISS 7  
FILE LAST UPDATED: 12 Aug 2002 (20020812/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

=> s l4

L5 28254 L4

=> s l5 and isoflavones

2454 ISOFLAVONES

L6 1459 L5 AND ISOFLAVONES

=> s l6/proc

28254 L4

1 ISOFLAVONES/CT

3189134 PROC/RL

0 ISOFLAVONES/PROC

(ISOFLAVONES/CT (L) PROC/RL)

L7 0 ((L4) AND ISOFLAVONES/PROC)

=> s l6/prep

28254 L4

1 ISOFLAVONES/CT

2897488 PREP/RL

0 ISOFLAVONES/PREP

(ISOFLAVONES/CT (L) PREP/RL)

L8 0 ((L4) AND ISOFLAVONES/PREP)

=> s l5/proc

FIELD CODES CANNOT BE CHANGED HERE

You may have tried to apply a field code to a term that already has a field code. You can only add a field code to a term that has no field code appended to it.

=> log y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

14.47

32.20

STN INTERNATIONAL LOGOFF AT 10:26:40 ON 13 AUG 2002

130

09/889,701

09889701

Page 1

08/13/2002

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PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 09:31:56 ON 13 AUG 2002

Golam Shameem

=&gt;

Uploading

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE

Do you want to switch to the Registry File?

Choice (Y/n):

Switching to the Registry File...

Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=&gt; FILE REGISTRY

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 09:32:15 ON 13 AUG 2002

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<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=&gt;

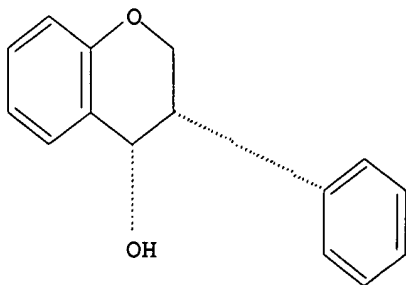
Uploading 09889701.str

L1 STRUCTURE UPLOADED

=&gt; d l1

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

Golam Shameem

=> s l1

SAMPLE SEARCH INITIATED 09:32:32 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 604 TO ITERATE

100.0% PROCESSED 604 ITERATIONS  
SEARCH TIME: 00.00.01

11 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 10606 TO 13554  
PROJECTED ANSWERS: 21 TO 417

L2 11 SEA SSS SAM L1

=> ~~FIL CAPLUS~~

~~COST IN U.S. DOLLARS~~

SINCE FILE	TOTAL
ENTRY	SESSION
0.38	0.59

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 09:32:42 ON 13 AUG 2002  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
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FILE COVERS 1907 - 13 Aug 2002 VOL 137 ISS 7  
FILE LAST UPDATED: 12 Aug 2002 (20020812/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

=> s l1

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...  
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 09:32:47 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 604 TO ITERATE

100.0% PROCESSED 604 ITERATIONS  
SEARCH TIME: 00.00.01

11 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 10606 TO 13554  
PROJECTED ANSWERS: 21 TO 417

L3 11 SEA SSS SAM L1

L4 8 L3

=> s l3/prep

8 L3  
2897488 PREP/RL

L5 5 L3/PREP  
(L3 (L) PREP/RL)

=> s l3/proc

8 L3  
3189134 PROC/RL

L6 0 L3/PROC  
(L3 (L) PROC/RL)

=> s l5 and hydrogenation

147967 HYDROGENATION  
1893 HYDROGENATIONS  
148239 HYDROGENATION

(HYDROGENATION OR HYDROGENATIONS)

L7 2 L5 AND HYDROGENATION

=> d ibib abs hitstr l7

L7 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2000:592710 CAPLUS

DOCUMENT NUMBER: 133:177059

TITLE: Preparation of isoflavone derivatives

INVENTOR(S): Heaton, Andrew; Kumar, Naresh

PATENT ASSIGNEE(S): Novogen Research Pty. Ltd., Australia

SOURCE: PCT Int. Appl., 55 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000049009	A1	20000824	WO 2000-AU103	20000215
W:	AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			

BR 2000008222

A

20011030

BR 2000-8222

20000215

EP 1153020

A1

20011114

EP 2000-904727

20000215

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
IE, SI, LT, LV, FI, RO

NO 2001003945

A

20010814

NO 2001-3945

20010814

PRIORITY APPLN. INFO.:

AU 1999-8685

A

19990215

WO 2000-AU103

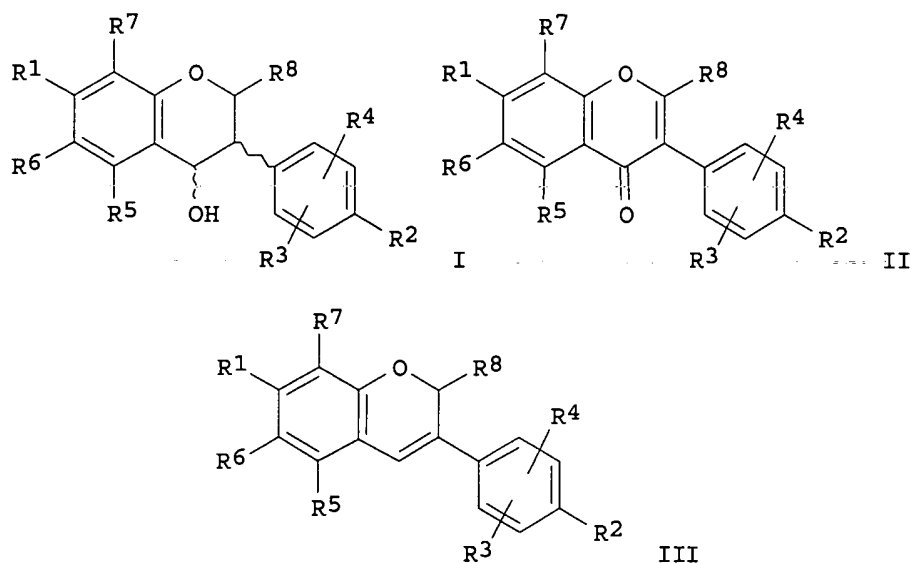
W

20000215

OTHER SOURCE(S):

MARPAT 133:177059

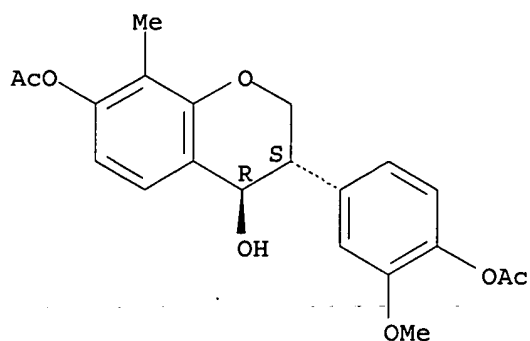
GI



- AB Isoflavone derivs., such as I, II, and III [R1-8 = H, OH, SH, NH<sub>2</sub>, NO<sub>2</sub>, alkyl, haloalkyl, aryl, arylalkyl, alkylthio, alkylamino, dialkylamino, halo, alkyloxy, aryloxy, acyloxy, alkylsulfinyloxy, arylsulfinyloxy, etc.], were prepd. Thus, daidzein diacetate was prepd. in 83% yield by acetylation of daidzein with acetic anhydride in pyridine. Methods for the **hydrogenation** of isoflavones are described which provide access to workable quantities of isoflavan-4-ols, isoflav-3-enes, and isoflavans. The isoflavone derivs. can be obtained in high purity and in near quant. yields while employing pharmaceutically acceptable reagents and solvents.
- IT **288266-89-7P**  
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP** (**Preparation**); RACT (Reactant or reagent)  
(prepn. of isoflavone derivs.)
- RN 288266-89-7 CAPLUS
- CN 2H-1-Benzopyran-4,7-diol, 3-[4-(acetyloxy)-3-methoxyphenyl]-3,4-dihydro-8-methyl-, 7-acetate, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.





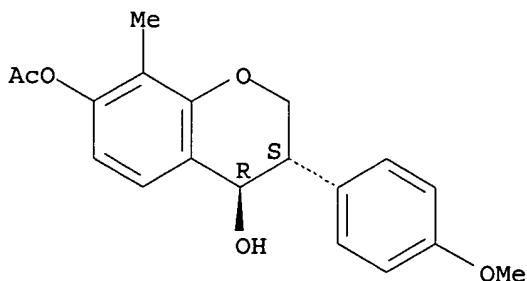
IT 288266-88-6P

RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use);  
BIOL (Biological study); **PREP (Preparation)**; RACT (Reactant or  
reagent); USES (Uses)  
(prepn. of isoflavone derivs.)

RN 288266-88-6 CAPLUS

CN 2H-1-Benzopyran-4,7-diol, 3,4-dihydro-3-(4-methoxyphenyl)-8-methyl-,  
7-acetate, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



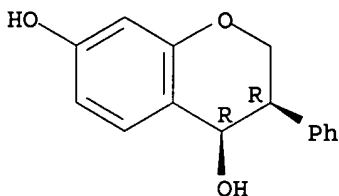
IT 288267-21-0P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological  
study); **PREP (Preparation)**; USES (Uses)  
(prepn. of isoflavone derivs.)

RN 288267-21-0 CAPLUS

CN 2H-1-Benzopyran-4,7-diol, 3,4-dihydro-3-phenyl-, (3R,4R)-rel- (9CI) (CA  
INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT:

14

THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs hitstr l5

L5 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2000:592710 CAPLUS

DOCUMENT NUMBER: 133:177059

TITLE: Preparation of isoflavone derivatives

INVENTOR(S): Heaton, Andrew; Kumar, Naresh

PATENT ASSIGNEE(S): Novogen Research Pty. Ltd., Australia

SOURCE: PCT Int. Appl., 55 pp.

CODEN: PIXXD2

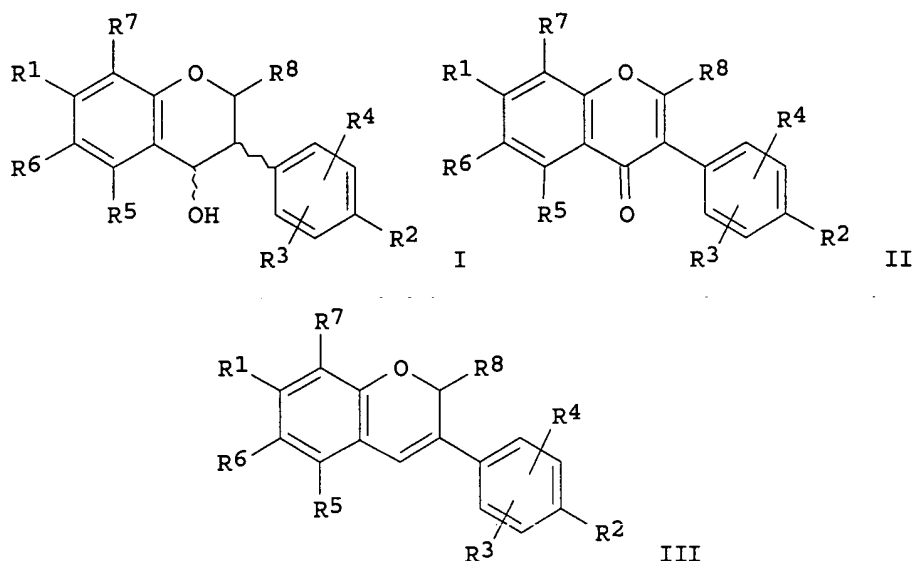
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

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PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000049009	A1	20000824	WO 2000-AU103	20000215
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RW:	GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
BR 2000008222	A	20011030	BR 2000-8222	20000215
EP 1153020	A1	20011114	EP 2000-904727	20000215
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO			
NO 2001003945	A	20010814	NO 2001-3945	20010814
PRIORITY APPLN. INFO.:			AU 1999-8685	A 19990215
			WO 2000-AU103	W 20000215
OTHER SOURCE(S):	MARPAT 133:177059			
GI				



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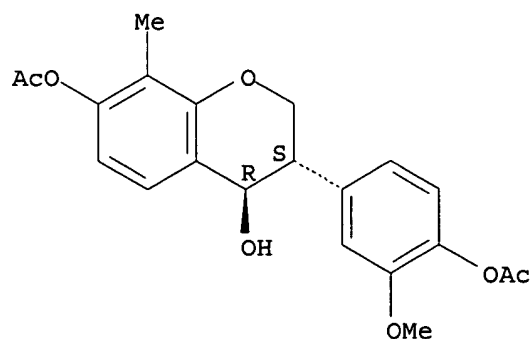
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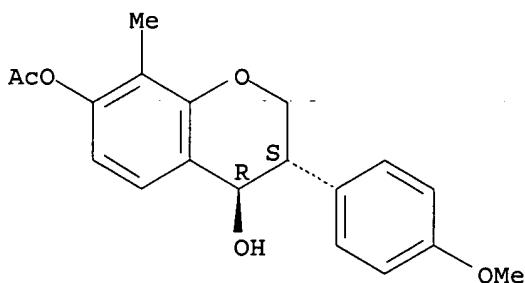
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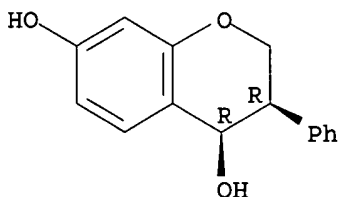
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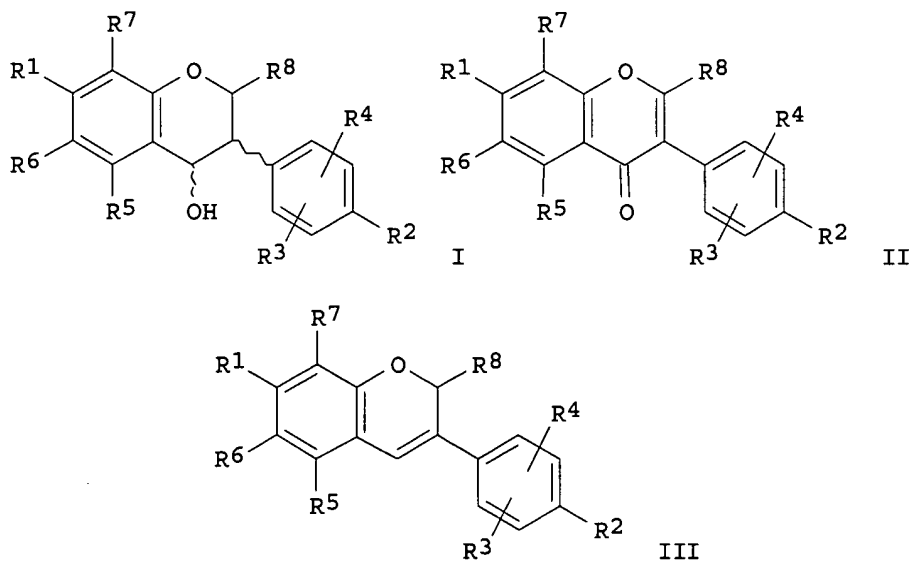
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

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WO 2000049009 A1 20000824 WO 2000-AU103 20000215  
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM  
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG  
BR 2000008222 A 20011030 BR 2000-8222 20000215  
EP 1153020 A1 20011114 EP 2000-904727 20000215  
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO  
NO 2001003945 A 20010814 NO 2001-3945 20010814  
PRIORITY APPLN. INFO.: AU 1999-8685 A 19990215  
WO 2000-AU103 W 20000215  
OTHER SOURCE(S): MARPAT 133:177059  
GI



AB Isoflavone derivs., such as I, II, and III [R1-8 = H, OH, SH, NH<sub>2</sub>, NO<sub>2</sub>, alkyl, haloalkyl, aryl, arylalkyl, alkylthio, alkylamino, dialkylamino, halo, alkyloxy, aryloxy, acyloxy, alkylsulfinyloxy, arylsulfinyloxy, etc.], were prepd. Thus, daidzein diacetate was prepd. in 83% yield by acetylation of daidzein with acetic anhydride in pyridine. Methods for the hydrogenation of isoflavones are described which provide access to workable quantities of isoflavan-4-ols, isoflav-3-enes, and isoflavans. The isoflavone derivs. can be obtained in high purity and in near quant. yields while employing pharmaceutically acceptable reagents and solvents.

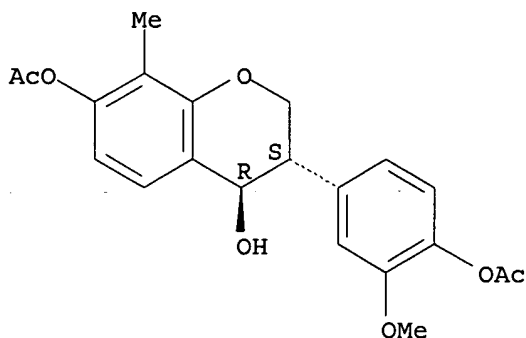
IT 288266-89-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. of isoflavone derivs.)

RN 288266-89-7 CAPLUS

CN 2H-1-Benzopyran-4,7-diol, 3-[4-(acetyloxy)-3-methoxyphenyl]-3,4-dihydro-8-methyl-, 7-acetate, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



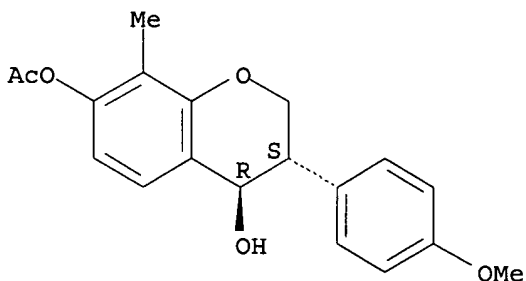
IT 288266-88-6P

RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(prepn. of isoflavone derivs.)

RN 288266-88-6 CAPLUS

CN 2H-1-Benzopyran-4,7-diol, 3-(4-methoxyphenyl)-8-methyl-, 7-acetate, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



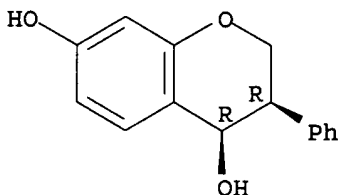
IT 288267-21-0P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of isoflavone derivs.)

RN 288267-21-0 CAPLUS

CN 2H-1-Benzopyran-4,7-diol, 3-phenyl-, (3R,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1998:402432 CAPLUS

DOCUMENT NUMBER: 129:81667

TITLE: Novel benzopyran and thiochroman derivatives useful as antiestrogens

INVENTOR(S): Jo, Jae Chon; Park, Sung Dae; Lim, Hyun Suk; Kim, Ju Su; Kim, Sung Jin; Morikawa, Kazumi; Kanbe, Yoshitake; Nishimoto, Masahiro; Kim, Myung-hwa

PATENT ASSIGNEE(S): C & C Research Laboratories, S. Korea; Jo, Jae Chon; Park, Sung Dae; Lim, Hyun Suk; Kim, Ju Su; Kim, Sung Jin; Morikawa, Kazumi; Kanbe, Yoshitake; Nishimoto, Masahiro; Kim, Myung-Hwa

SOURCE: PCT Int. Appl., 125 pp.

CODEN: PIXXD2

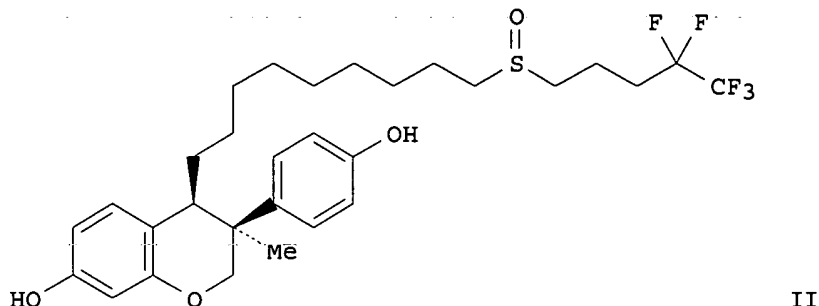
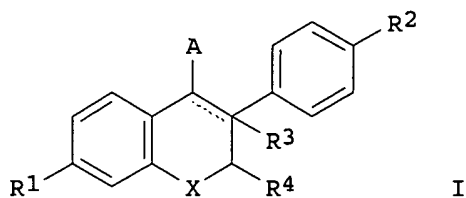
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9825916	A1	19980618	WO 1997-KR265	19971213
W:	AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG			
AU 9854134	A1	19980703	AU 1998-54134	19971213
AU 722089	B2	20000720		
EP 944613	A1	19990929	EP 1997-947971	19971213
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI			
CN 1244863	A	20000216	CN 1997-181472	19971213
JP 2000507620	T2	20000620	JP 1998-526521	19971213
JP 3251946	B2	20020128		
US 6153768	A	20001128	US 1999-319616	19990608
PRIORITY APPLN. INFO.:			KR 1996-65301	A 19961213
			KR 1997-26915	A 19970624
			WO 1997-KR265	W 19971213
OTHER SOURCE(S):		MARPAT 129:81667		
GI				



AB The invention relates to novel benzopyran derivs. having anti-estrogenic activity. More specifically, the invention relates to novel benzopyran and thiochroman derivs. I and pharmaceutically acceptable salts thereof [in which the dashed line = optional pi bond; R1, R2 = H, OH, or OR; R = acyl or alkyl; R3 = H, alkyl, haloalkyl, or null when R3 is absent; R4 = H or alkyl; A = (CH2)mSONR5, C6H4O(CH2)mSONR5, C6H4O(CH2)mNR6R7, (CH2)mSON(CH2)pNR6R7; R5, R6, and R7 = H, alkyl, haloalkyl, alkenyl, or haloalkenyl; or NR6R7 = 4- to 8-membered heterocyclic ring which can be substituted with R5; X = O, S, or NR8; R8 = H or alkyl; m = 2-15; n = 0-2; and p = 0-4]. Also disclosed are a prepn. process, and antiestrogenic pharmaceutical compns. which contains I as an active component. Examples include over 80 syntheses and 4 bioassays. For example, compd. II was prepd. by a 7-step sequence involving: (1) double-O-methoxymethylation and 3-methylation of 7-hydroxy-3-(4-hydroxyphenyl)-2,3-dihydro-4H-benzopyran-4-one (66%), (2) 4-alkynylation with HC.tplbond.C(CH2)7OSiMe2CMe3 (100%), (3) desilylation (33%), O-tosylation (88%), thioetherification (97%), deprotection of OH groups (66%), and S-oxidn. with NaIO4 (73%). The antiestrogenic and MCF-7 cell growth-inhibiting activities of II were comparable or superior to the related antiestrogen ZM-189154, and the side effect of decreased bone mineral d. in II was not only reduced but to some extent reversed.

IT 209324-98-1P

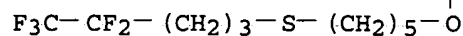
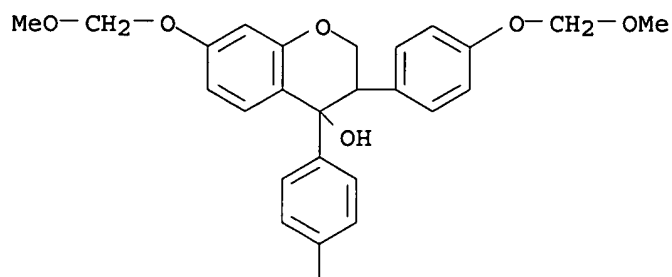
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP** (Preparation); RACT (Reactant or reagent)

(prepn. of benzopyran and thiochroman derivs. as antiestrogens)

RN 209324-98-1 CAPLUS

CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-7-(methoxymethoxy)-3-[4-(methoxymethoxy)phenyl]-4-[4-[5-[(4,4,5,5,5-pentafluoropentyl)thio]pentyl]oxy]phenyl]- (9CI) (CA INDEX NAME)





L5 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1986:148589 CAPLUS

DOCUMENT NUMBER: 104:148589

TITLE: The chemistry of the 'insoluble red woods'. Part 16.  
Some further observations on the condensation of  
isoflavylium salts with 1,3-diphenylpropenes

AUTHOR(S): Afonya, Theophilus C. A.; Epelle, Faithwin B. M.;  
Osman, Soad A. A.; Whalley, W. Basil

CORPORATE SOURCE: Sch. Pharm., London, WC1N 1AX, UK

SOURCE: J. Chem. Res., Synop. (1985), (10), 305

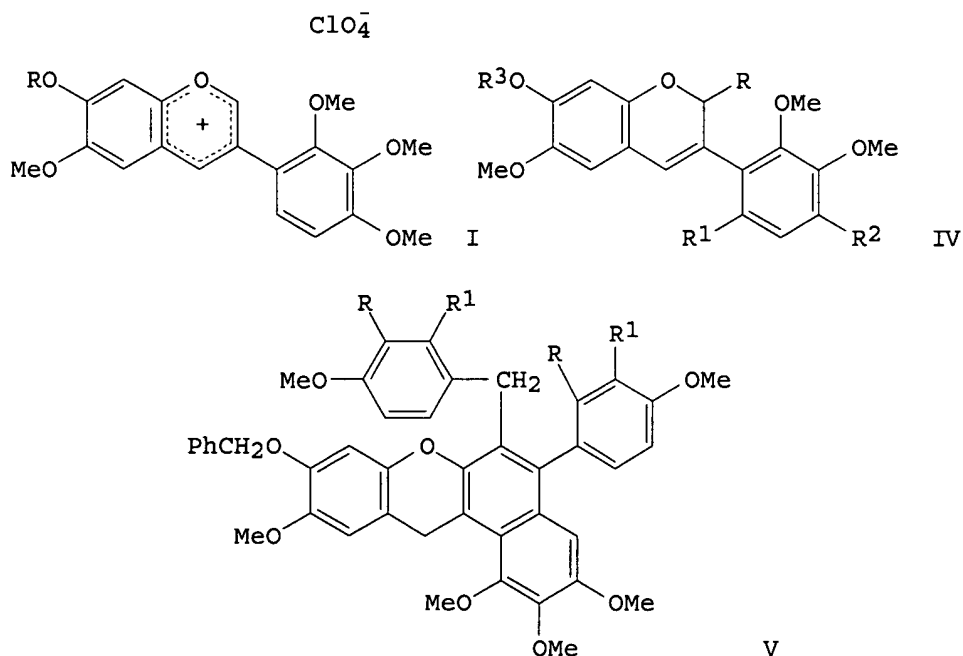
CODEN: JRPSDC; ISSN: 0308-2342

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 104:148589

GI



AB Condensation of isoflavylium perchlorate I (R = CH<sub>2</sub>Ph) (II) with

Golam Shameem

3,4-(MeO)2C6H3CH:CHCH2C6H3(OMe)2-2,4 (III) in refluxing MeCN for 3 h gave isoflavene IV (R = R1 = H, R2 = OMe, R3 = CH2Ph) and benzoxanthene V (R = H, R1 = OMe). Similar reaction of II with 2,4-(MeO)2C6H3CH:CHCH2C6H3(OMe)2-3,4 (VI) gave isoflavene IV (R = R2 = OMe, R1 = H; R = R2 = H, R1 = OMe; R3 = CH2Ph) and benzoxanthene V (R = OMe, R1 = H). Analogous reaction of I (R = Me) with III or VI gave only the isoflavene IV (R = R2 = OMe, R1 = H, R3 = Me). The preps. of the starting materials are reported.

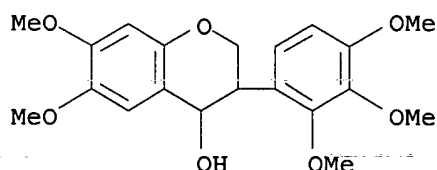
IT 100753-48-8P

RL: RCT (Reactant); SPN (Synthetic preparation); **PREP**  
(Preparation)

(prepn. and elimination reaction of, isoflavylium salt by)

RN 100753-48-8 CAPLUS

CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-6,7-dimethoxy-3-(2,3,4-trimethoxyphenyl)-  
(9CI) (CA INDEX NAME)



L5 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1971:476524 CAPLUS

DOCUMENT NUMBER: 75:76524

TITLE: Reactions of isoflavanones with Grignard reagents.  
Synthesis of estrogenic and antiestrogenic active  
isoflavanoids

AUTHOR(S): Irmscher, Klaus; Borck, Joachim

CORPORATE SOURCE: Chem. Forsch. E. Merck, Darmstadt, Ger.

SOURCE: Justus Liebigs Ann. Chem. (1971), 744, 164-77

CODEN: JLACBF

DOCUMENT TYPE: Journal

LANGUAGE: German

GI For diagram(s), see printed CA Issue.

AB Grignard reaction of isoflavanones or 2-ethyl-7-methoxyisoflavanones (I) gave 4-aryl-4-isoflavanols or 2-ethyl-7-methoxy-4-aryl-4-isoflavanols (II), resp., which were dehydrated to 4-aryl-3-isoflavenes. Depending on the reaction conditions, the constitution of the isoflavanone, and the Grignard reagent, the C-2 atom of the isoflavanone was also attached in some cases to give .beta.-aryl-.alpha.-phenyl-2-hydroxypropiofenones with ring opening. The mechanism of the ring opening involving an .alpha.-methylene ketone was discussed.

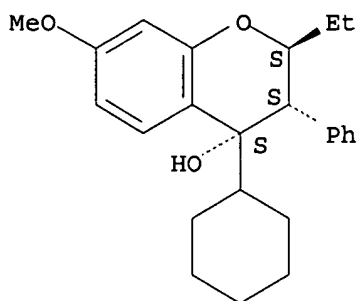
IT 33103-17-2P

RL: SPN (Synthetic preparation); **PREP** (Preparation)  
(prepn. of)

RN 33103-17-2 CAPLUS

CN 4-Isiflavanol, 4-cyclohexyl-2-ethyl-7-methoxy-, stereoisomer (8CI) (CA  
INDEX NAME)

Relative stereochemistry.



L5 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1967:28657 CAPLUS

DOCUMENT NUMBER: 66:28657

TITLE: 3,4-Diaryl-4-chromanols and 3,4-diaryl-3-chromenes

PATENT ASSIGNEE(S): Merck, E., A.-G.

SOURCE: Neth. Appl., 26 pp.

CODEN: NAXXAN

DOCUMENT TYPE: Patent

LANGUAGE: Dutch

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
NL 6517021		19660704		

PRIORITY APPLN. INFO.: DE 19650102

GI For diagram(s), see printed CA Issue.

AB The title compds. are prepd. by condensation of 3-aryl-4-chromanones with organo-metallic compds. followed by dehydration. A soln. of 0.66 g. I (R = R1 = H) (IV) in 30 ml. abs. C6H6 is dropped to a soln. of p-MeOC6H4MgBr (from 2.2 g. p-MeOC6H4Br and 0.23 g. Mg) in abs. Et2O, the Et2O distd., and the mixt. refluxed 16 hrs., cooled, decompd. with 100 ml. 10% HCl, and the C6H6 layer sped. to yield II (R = R1 = H, R2 = MeO), m. 144-5.degree. (CHCl3-Et2O). Likewise, the following II are prepd. (R, R1, R2, and m.p. given): H, H, H, 127-31.degree. (V); Et, H, H, 121-3.degree.; H, MeO, H, 151-2.degree.; Et, MeO, H, 158.degree. and 105.degree. (2 isomers); Et, MeO, MeO, 105-6.degree.; H, H, PhCH2O, 122-3.degree. (VI); Et, MeO, PhCH2O, 126.degree. and 137.degree. (2 isomers). To a soln. of IV (0.68 g.) in 30 ml. abs. C6H6 is added dropwise a soln. of PhLi (4 millimoles) in Et2O. After the same treatment as above V is isolated; when the mixt. is heated 5 hrs. after adding 10% HCl, III (R = R1 = R2 = H) is obtained, m. 130-2.degree. (Et2O-petroleum ether). Similarly prepd. are III (R = R1 = H, R2 = MeO), m. 119-21.degree., and III (R = H, R1 = R2 = MeO), m. 162-5.degree.. By treating I [R = H, R1 = tetrahydropyranyl-2-oxy (Q)] with PhMgBr as described, but decompg. with NH4Cl soln., II (R = R2 = H, R1 = Q) is obtained, while from the alk. washing fluid some II (R = R2 = H, R1 = OH) (VIII) is isolated). Similarly is prepd. from IV and p-QC6H4MgBr II (R = R1 = H, R2 = Q) (IX). VII (2 g.) is refluxed 2.5 hrs. in 50 ml. 5% HCl in dil. EtOH, the mixt. cooled and extd. with CHCl3 to yield III (R = R2 = H, R1 = OH) (X); similarly are obtained III (R = R1 = H, R2 = OH) (XI), m. 188-9.degree., from IX, and III (R = H, R1 = MeO, R2 = OH), m. 118.degree.. A soln. of 2 g. VI in 200 ml. EtOAc is hydrogenated at room temp. over 5% Pd-C, filtered, concd., the residue chromatographed on SiO2, and eluted with C6H6 to yield II (R = R1 = H, R2 = OH) (XII); similarly are prepd. II (R = H, R1 = MeO, R2 = OH), m.

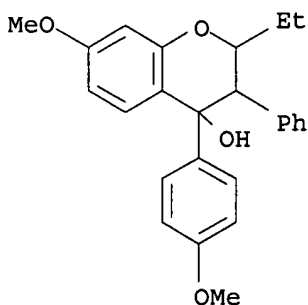
173.degree. and II (R = Et, R1 = MeO, R2 = OH), m. 112.degree. and 150-2.degree. (2 isomers). XII (0.99 g.) is heated 5 hrs. at 100.degree. with a mixt. of 0.7 ml. H2SO4 and 13 ml. dioxane, cooled, poured on ice, extd. with CHCl3, the ext. concd., and the residue crystd. from Et2O-petroleum ether to give XI, m. 188-9.degree.. X (0.5 g.) in 10 ml. Me2CO is boiled 24 hrs. in N with 0.3 g. ClCH2CO2Et and 0.35 g. anhyd. K2CO3, concd., and extd. with CH2Cl2 to yield III (R = R2 = H, R1 = EtO2CCH2O) (XIII). XI (1 g.), 4 g. 2-pyrrolidinonethyl chloride, 1.2 g. dry K2CO3, and 40 ml. abs. Me2CO are stirred and boiled 20 hrs., concd., the residue dild. with H2O and Et2O, the Et2O layer sepd. dried, on KOH, concd., and the residue chromatographed on Al2O3 and eluted with CHCl3 to give III (R = R1 = H, R2 = 2-pyrrolidinoethoxy), m. 98-9.degree. (Me2CO-Et2O). X (1 g.), 5 ml. C5H5N, and 5 ml. Ac2O are heated 5 hrs. at 50.degree., cooled, and extd. with CHCl3 to yield III (R = R2 = H, R1 = AcO). To a soln. of 21 ml. POCl3 in 210 ml. abs. C5H5N is added with stirring in 15 min. at 5.degree. a soln. of 7.8 g. X in 105 ml. C5H5N; after 15 hrs. at room temp. the mixt. is poured on a mixt. of 3 kg. ice and 300 ml. concd. HCl, heated at 100.degree. for 90 min., cooled, extd. with EtOAc, the ext. washed with HCl, dried on Na2SO4, filtered, and concd. to yield the phosphate of X. H2NSO3H (6 g.) and 7.5 g. X are suspended in 5 ml. abs. C5H5N, stirred 90 min. at 100.degree., cooled, filtered, the filter washed with C5H5N, the filtrate extd. with abs. Et2O, the residue dried in vacuo, 75 ml. 12% NaOH and 53 ml. C5H5N added and shaken for 5 min.; the upper C5H5N layer washed with Et2O, MeOH added and concd., and the residue crystd. from MeOH to yield III (R = R2 = H, R1 = OSO3Na). XIII (2 g.) is refluxed 3 hrs. with 30 ml. 2N KOH in EtOH, and the soln. acidified to yield III (R = R2 = H, R1 = HO2CCH2O); XIII (3.5 g.) is refluxed 6 hrs. in a mixt. of 2 g. pyrrolidine and 10 ml. abs. C6H6, and the soln. concd. to yield III (R = R2 = H, R1 = QCOCH2O) (Q = pyrrolidino). II and III have antigonadotropic and contraceptive effects.

IT 13417-66-8P 13417-74-8P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

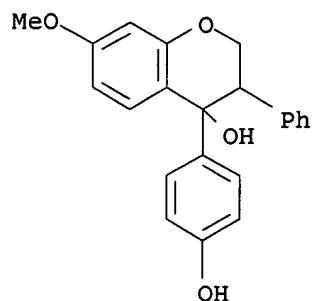
RN 13417-66-8 CAPLUS

CN 4-Chromanol, 2-ethyl-7-methoxy-4-(p-methoxyphenyl)-3-phenyl- (8CI) (CA INDEX NAME)



RN 13417-74-8 CAPLUS

CN 4-Chromanol, 4-(p-hydroxyphenyl)-7-methoxy-3-phenyl- (8CI) (CA INDEX NAME)



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L7 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2000:592710 CAPLUS

DOCUMENT NUMBER: 133:177059

TITLE: Preparation of isoflavone derivatives

INVENTOR(S): Heaton, Andrew; Kumar, Naresh

PATENT ASSIGNEE(S): Novogen Research Pty. Ltd., Australia

SOURCE: PCT Int. Appl., 55 pp.

CODEN: PIXXD2

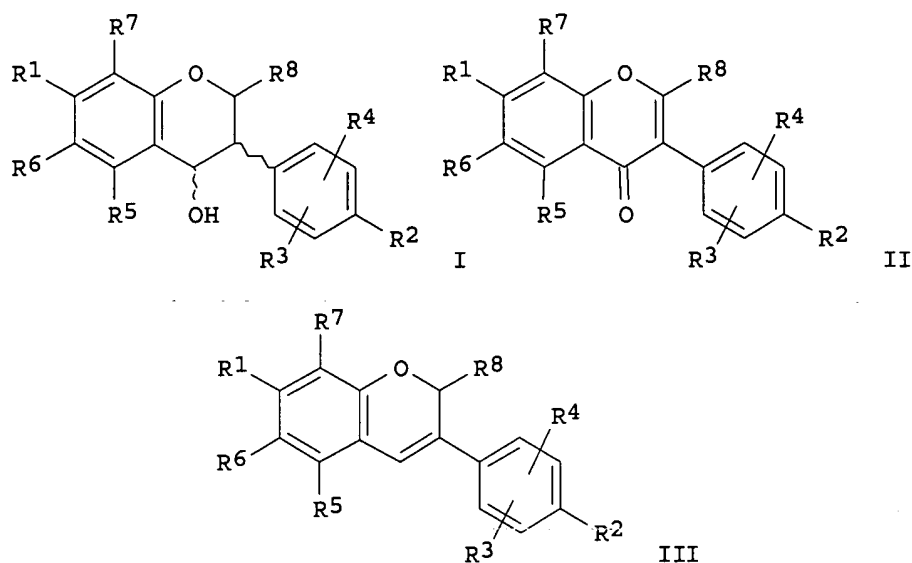
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000049009	A1	20000824	WO 2000-AU103	20000215
W:	AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
BR 2000008222	A	20011030	BR 2000-8222	20000215
EP 1153020	A1	20011114	EP 2000-904727	20000215
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO			
NO 2001003945	A	20010814	NO 2001-3945	20010814
PRIORITY APPLN. INFO.:			AU 1999-8685	A 19990215
			WO 2000-AU103	W 20000215
OTHER SOURCE(S):	MARPAT 133:177059			
GI				



AB Isoflavone derivs., such as I, II, and III [R1-8 = H, OH, SH, NH<sub>2</sub>, NO<sub>2</sub>, alkyl, haloalkyl, aryl, arylalkyl, alkylthio, alkylamino, dialkylamino, halo, alkyloxy, aryloxy, acyloxy, alkylsulfinyloxy, arylsulfinyloxy, etc.], were prepd. Thus, daidzein diacetate was prepd. in 83% yield by acetylation of daidzein with acetic anhydride in pyridine. Methods for the **hydrogenation** of isoflavones are described which provide access to workable quantities of isoflavan-4-ols, isoflav-3-enes, and isoflavans. The isoflavone derivs. can be obtained in high purity and in near quant. yields while employing pharmaceutically acceptable reagents and solvents.

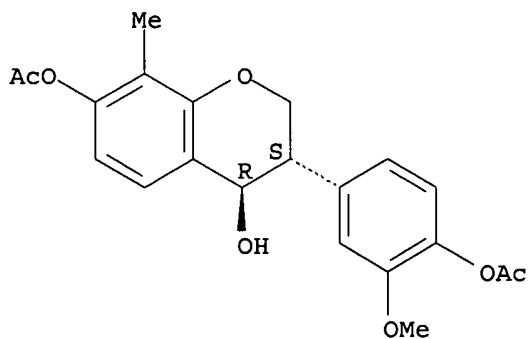
IT 288266-89-7P

RL: RCT (Reactant); SPN (Synthetic preparation); **PREP** (Preparation); RACT (Reactant or reagent)  
(prepn. of isoflavone derivs.)

RN 288266-89-7 CAPLUS

CN 2H-1-Benzopyran-4,7-diol, 3-[4-(acetyloxy)-3-methoxyphenyl]-3,4-dihydro-8-methyl-, 7-acetate, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 288266-88-6P

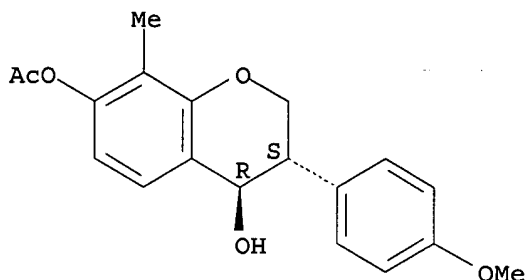
RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use);

BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(prepn. of isoflavone derivs.)

RN 288266-88-6 CAPLUS

CN 2H-1-Benzopyran-4,7-diol, 3,4-dihydro-3-(4-methoxyphenyl)-8-methyl-,  
7-acetate, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



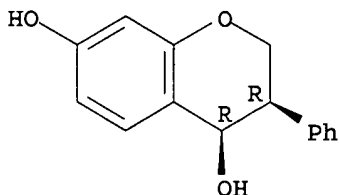
IT 288267-21-0P

RL: SPN= (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of isoflavone derivs.)

RN 288267-21-0 CAPLUS

CN 2H-1-Benzopyran-4,7-diol, 3,4-dihydro-3-phenyl-, (3R,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1986:148589 CAPLUS

DOCUMENT NUMBER: 104:148589

TITLE: The chemistry of the 'insoluble red woods'. Part 16.  
Some further observations on the condensation of  
isoflavylum salts with 1,3-diphenylpropenes

AUTHOR(S): Afonya, Theophilus C. A.; Epelle, Faithwin B. M.;  
Osman, Soad A. A.; Whalley, W. Basil

CORPORATE SOURCE: Sch. Pharm., London, WC1N 1AX, UK

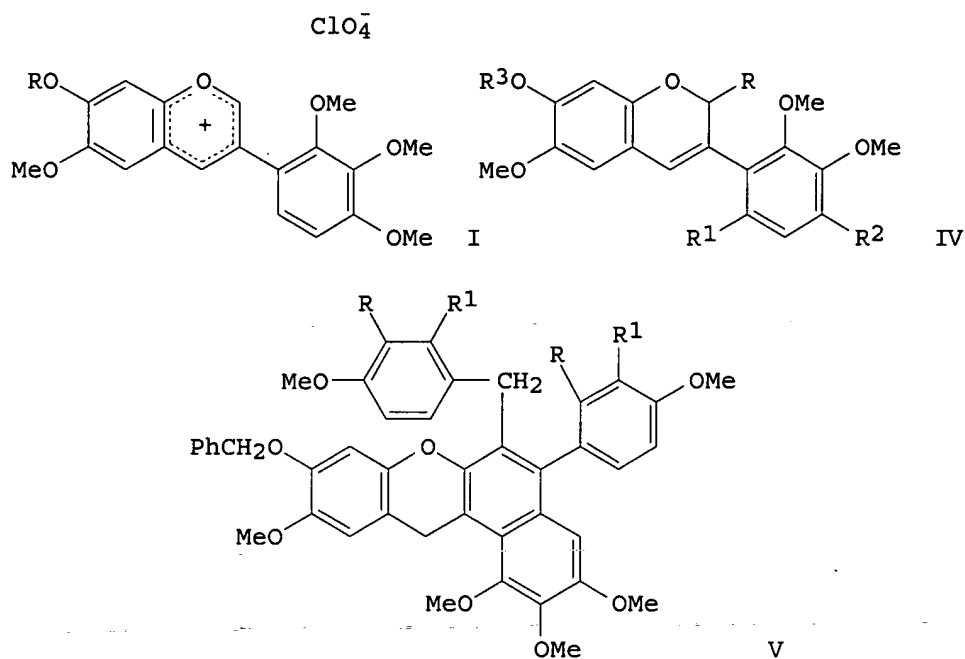
SOURCE: J. Chem. Res., Synop. (1985), (10), 305  
CODEN: JRPSDC; ISSN: 0308-2342

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 104:148589

GI



AB Condensation of isoflavylium perchlorate I ( $R = \text{CH}_2\text{Ph}$ ) (II) with 3,4-(MeO) $2\text{C}_6\text{H}_3\text{CH}:\text{CHCH}_2\text{C}_6\text{H}_3(\text{OMe})_{2-2,4}$  (III) in refluxing MeCN for 3 h gave isoflavene IV ( $R = R_1 = \text{H}$ ,  $R_2 = \text{OMe}$ ,  $R_3 = \text{CH}_2\text{Ph}$ ) and benzoxanthene V ( $R = \text{H}$ ,  $R_1 = \text{OMe}$ ). Similar reaction of II with 2,4-(MeO) $2\text{C}_6\text{H}_3\text{CH}:\text{CHCH}_2\text{C}_6\text{H}_3(\text{OMe})_{2-3,4}$  (VI) gave isoflavene IV ( $R = R_2 = \text{OMe}$ ,  $R_1 = \text{H}$ ;  $R = R_2 = \text{H}$ ,  $R_1 = \text{OMe}$ ;  $R_3 = \text{CH}_2\text{Ph}$ ) and benzoxanthene V ( $R = \text{OMe}$ ,  $R_1 = \text{H}$ ). Analogous reaction of I ( $R = \text{Me}$ ) with III or VI gave only the isoflavene IV ( $R = R_2 = \text{OMe}$ ,  $R_1 = \text{H}$ ,  $R_3 = \text{Me}$ ). The preps. of the starting materials are reported.

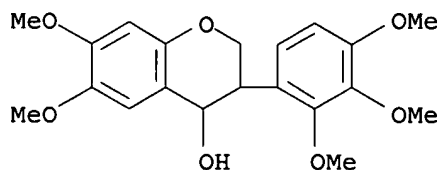
IT **100753-48-8P**

RL: RCT (Reactant); SPN (Synthetic preparation); **PREP**  
(Preparation)

(prepn. and elimination reaction of, isoflavylium salt by)

RN 100753-48-8 CAPLUS

CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-6,7-dimethoxy-3-(2,3,4-trimethoxyphenyl)-(9CI) (CA INDEX NAME)



=> log y

COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE

ENTRY

47.95

TOTAL

SESSION

49.32

Golam Shameem



09889701

Page 22

08/13/2002

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-5.58	-5.58

STN INTERNATIONAL LOGOFF AT 09:38:09 ON 13 AUG 2002

(130)

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:sssptal626gms

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* Welcome to STN International \* \* \* \* \*

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NEWS 2 Apr 08 "Ask CAS" for self-help around the clock  
NEWS 3 Apr 09 BEILSTEIN: Reload and Implementation of a New Subject Area  
NEWS 4 Apr 09 ZDB will be removed from STN  
NEWS 5 Apr 19 US Patent Applications available in IFICDB, IFIPAT, and IFIUDB  
NEWS 6 Apr 22 Records from IP.com available in CAPLUS, HCAPLUS, and ZCAPLUS  
NEWS 7 Apr 22 BIOSIS Gene Names now available in TOXCENTER  
NEWS 8 Apr 22 Federal Research in Progress (FEDRIP) now available  
NEWS 9 Jun 03 New e-mail delivery for search results now available  
NEWS 10 Jun 10 MEDLINE Reload  
NEWS 11 Jun 10 PCTFULL has been reloaded  
NEWS 12 Jul 02 FOREG no longer contains STANDARDS file segment  
NEWS 13 Jul 22 USAN to be reloaded July 28, 2002;  
saved answer sets no longer valid  
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NEWS 16 Aug 08 CANCERLIT reload  
NEWS 17 Aug 08 PHARMAMarketLetter(PHARMAML) - new on STN  
NEWS 18 Aug 08 NTIS has been reloaded and enhanced  
NEWS 19 Aug 09 JAPIO to be reloaded August 18, 2002  
  
NEWS EXPRESS February 1 CURRENT WINDOWS VERSION IS V6.0d,  
CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP),  
AND CURRENT DISCOVER FILE IS DATED 05 FEBRUARY 2002  
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FILE 'HOME' ENTERED AT 10:34:54 ON 13 AUG 2002

=> s flavone

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE

Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FIL REGISTRY

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 10:35:30 ON 13 AUG 2002

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STRUCTURE FILE UPDATES: 12 AUG 2002 HIGHEST RN 443729-39-3

DICTIONARY FILE UPDATES: 12 AUG 2002 HIGHEST RN 443729-39-3

TSCA INFORMATION NOW CURRENT THROUGH January 7, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:

<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> s flavone

6194 FLAVONE

1 FLAVONES

L1

6194 FLAVONE

(FLAVONE OR FLAVONES)

=> FIL CAPLUS

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

4.38

4.59

FILE 'CAPLUS' ENTERED AT 10:35:54 ON 13 AUG 2002

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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FILE COVERS 1907 - 13 Aug 2002 VOL 137 ISS 7  
FILE LAST UPDATED: 12 Aug 2002 (20020812/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

=> s l1

L2 28254 L1

=> s l1/proc

28254 L1  
3189134 PROC/RL  
L3 1943 L1/PROC  
(L1 (L) PROC/RL)

=> s l1/prep

28254 L1  
2897488 PREP/RL  
L4 3978 L1/PREP  
(L1 (L) PREP/RL)

=> s l3 and hydrogenation?

148247 HYDROGENATION?  
L5 3 L3 AND HYDROGENATION?

=> d ibib abs hitstr l5 tot

L5 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1995:787564 CAPLUS

DOCUMENT NUMBER: 123:226958

TITLE: A urinary profile study of dietary phytoestrogens. The identification and mode of metabolism of new isoflavonoids

AUTHOR(S): Joannou, G. E.; Kelly, G. E.; Reeder, A. Y.; Waring, M.; Nelson, C.

CORPORATE SOURCE: Department of Metabolic Mass Spectrometry, Royal Prince Alfred Hospital, Sydney, 2050, Australia

SOURCE: J. Steroid Biochem. Mol. Biol. (1995), 54(3/4), 167-84  
CODEN: JSBBEZ; ISSN: 0960-0760

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The metabolic fate of the dietary isoflavones daidzein and genistein was investigated in human volunteers challenged with soya. Urinary diphenols, isolated by partition chromatog. on Sephadex LH-20, were characterized and identified by profile capillary gas chromatog. (GC) and electron ionization mass spectrometry (GC-EIMS) anal. of the trimethylsilyl ether (TMS) derivs. Novel isoflavonic phytoestrogens found in the urine of volunteers were those of tetrahydrodaidzein, dihydrogenistein, 6'-hydroxy-O-demethylangolensin and 2-dehydro-O-demethylangolensin. Other known diphenols identified were those of equol, dihydrodaidzein, O-demethylangolensin, daidzein, genistein, glycitein, and the lignan enterolactone. Two other urinary isomers with a fragmentation pattern

closely resembling that of the persilylated TMS ethers of cis/trans-isomers of tetrahydrodaidzein, were characterized based on the elucidation of fragments assocd. with the loss of a nonphenolic-OTMS functional group in ring-C. These are fragments presented in the persilylated mass spectra of isoflavan-4-ols and isoflav-3-ene-4-ols, demonstrated here by a combination of simple and tandem mass spectrometry study of the deuterated persilylated TMS ethers of dihydrodaidzein. In a similar study the authors also present the data on the structural identification and fragment elucidation of the keto/enol tautomers of the TMS ether derivs. of the dihydro derivs. of daidzein and genistein, obsd. in the urine of volunteers and considered probable products of the derivatization process. Finally, the GC and GC-MS data of two unknown isoflavonoids and that of a lignan-like compd. are presented together with those of dihydrodaidzein, dihydrogenistein, tetrahydrodaidzein and 2-dehydro-O-demethylangolensin. The latter four were obtained here as products of small scale chem. synthesis in a preliminary study on the tentative identification of urinary isoflavonoids in human volunteers challenged with soya.

IT 446-72-0, Genistein 486-66-8, Daidzein

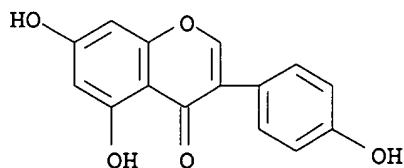
RL: BPR (Biological process); RCT (Reactant); BIOL (Biological study);

PROC (Process)

(metabolic fate of human dietary isoflavones and hydrogenation of)

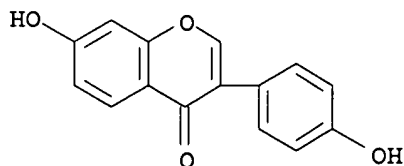
RN 446-72-0 CAPLUS

CN 4H-1-Benzopyran-4-one, 5,7-dihydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



RN 486-66-8 CAPLUS

CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1983:605536 CAPLUS

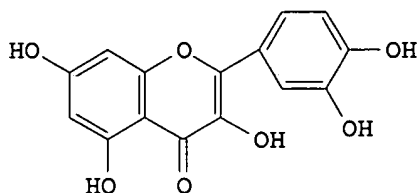
DOCUMENT NUMBER: 99:205536

TITLE: Studies on drug metabolism by use of isotopes. XXVII: Urinary metabolites of rutin in rats and the role of intestinal microflora in the metabolism of rutin

AUTHOR(S): Baba, Shigeo; Furuta, Takashi; Fujioka, Minoru; Goromaru, Tsuyoshi

CORPORATE SOURCE: Tokyo Coll. Pharm., Hachioji, 192-03, Japan

SOURCE: J. Pharm. Sci. (1983), 72(10), 1155-8  
CODEN: JPMSAE; ISSN: 0022-3549  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB Anal. of urinary metabolites of orally administered rutin (I) [153-18-4] labeled with deuterium ([2',5',6'-2H]rutin (rutin-d) [78800-17-6]) was carried out by gas-liq chromatog.-mass spectroscopy. In rat urine, 3-hydroxyphenylacetic acid [621-37-4], 3-methoxy-4-hydroxyphenylacetic acid [34919-76-1], 3,4-dihydroxyphenylacetic acid [102-32-9], 3,4-dihydroxytoluene [452-86-8], and 3-(m-hydroxyphenyl)propionic acid [621-54-5] were identified as rutin metabolites and were differentiated from the corresponding endogeneous compds. Unchanged I and quercetin [117-39-5] were not present in the urine. Rutin-d was injected i.p. in rats, administered orally to neomycin-treated rats, and incubated in vitro with the intestinal contents of rats. The expts. suggested the involvement of intestinal microflora in the metab. of orally administered I.

IT 153-18-4

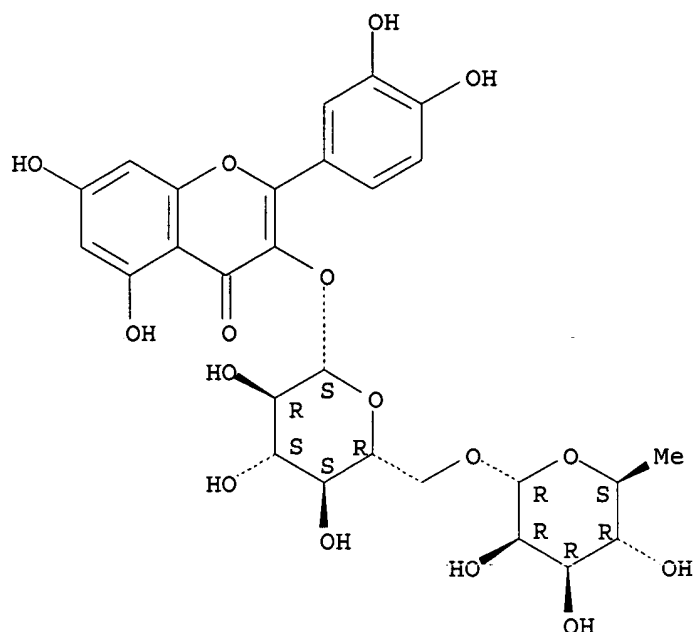
RL: BPR (Biological process); BIOL (Biological study); PROC (Process)

(metab. of, intestinal microorganisms in)

RN 153-18-4 CAPLUS

CN 4H-1-Benzopyran-4-one, 3-[[6-O-(6-deoxy-.alpha.-L-mannopyranosyl)-.beta.-D-glucopyranosyl]oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L5 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1980:140446 CAPLUS

DOCUMENT NUMBER: 92:140446

TITLE: Some derivatives of budlein A and B and the cytotoxic activity of substance A in two cell lines

AUTHOR(S): Roche, P.; Rosas, N.; Taboada, J.; Gonzalez Diddi, M.; Tellez, J.

CORPORATE SOURCE: Inst. Quim., Univ. Nac. Auton. Mexico, Mexico City, 20, Mex.

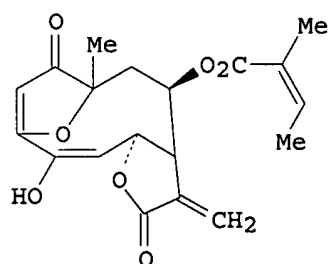
SOURCE: Rev. Latinoam. Quim. (1979), 10(4), 145-9

CODEN: RLAQA8; ISSN: 0370-5943

DOCUMENT TYPE: Journal

LANGUAGE: Spanish

GI



I

AB Budlein A (I) [59481-48-0], budlein B [60147-79-7], and salvigenin [19103-54-9] were isolated from *Viguiera* plants. Some derivs. of I (Me ether, chlorinated and hydrogenated products) and budlein B (Cope rearrangement product) were prepd. and identified. The cytotoxic activity of only 1 of the compds. (I) was evaluated. At 1-10  $\mu\text{g/mL}$ , I only slightly decreased the no. of mitosis in HEP-2 cell cultures (human

laryngeal carcinoma), whereas at 50 .mu.g/mL it inhibited cellular growth by 79%. For murine connective tissue cultures, I inhibited cellular growth by 83% at 1 .mu.g/mL and increased the no. of multinuclear cells by .apprx.5-fold.

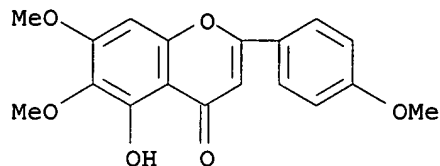
IT 19103-54-9

RL: PROC (Process)

(isolation of, from Viguiera)

RN 19103-54-9 CAPLUS

CN 4H-1-Benzopyran-4-one, 5-hydroxy-6,7-dimethoxy-2-(4-methoxyphenyl) - (9CI)  
(CA INDEX NAME)



=> s 13 and isoflavones

2454 ISOFLAVONES

L6 199 L3 AND ISOFLAVONES

=> s 16/proc

28254 L1

3189134 PROC/RL

1943 L1/PROC

(L1 (L) PROC/RL)

1 ISOFLAVONES/CT

3189134 PROC/RL

0 ISOFLAVONES/PROC

(ISOFLAVONES/CT (L) PROC/RL)

L7 0 ((L1/PROC) AND ISOFLAVONES/PROC)

=> s 16 and hydrogenation

147967 HYDROGENATION

1893 HYDROGENATIONS

148239 HYDROGENATION

(HYDROGENATION OR HYDROGENATIONS)

L8 1 L6 AND HYDROGENATION

=> d ibib abs hitstr tot

L8 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1995:787564 CAPLUS

DOCUMENT NUMBER: 123:226958

TITLE: A urinary profile study of dietary phytoestrogens. The identification and mode of metabolism of new isoflavonoids

AUTHOR(S): Joannou, G. E.; Kelly, G. E.; Reeder, A. Y.; Waring, M.; Nelson, C.

CORPORATE SOURCE: Department of Metabolic Mass Spectrometry, Royal Prince Alfred Hospital, Sydney, 2050, Australia

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CODEN: JSBBEZ; ISSN: 0960-0760

DOCUMENT TYPE: Journal



LANGUAGE: English

AB The metabolic fate of the dietary **isoflavones** daidzein and genistein was investigated in human volunteers challenged with soya. Urinary diphenols, isolated by partition chromatog. on Sephadex LH-20, were characterized and identified by profile capillary gas chromatog. (GC) and electron ionization mass spectrometry (GC-EIMS) anal. of the trimethylsilyl ether (TMS) derivs. Novel isoflavonic phytoestrogens found in the urine of volunteers were those of tetrahydrodaidzein, dihydrogenistein, 6'-hydroxy-O-demethylangolensin and 2-dehydro-O-demethylangolensin. Other known diphenols identified were those of equol, dihydrodaidzein, O-demethylangolensin, daidzein, genistein, glycitein, and the lignan enterolactone. Two other urinary isomers with a fragmentation pattern closely resembling that of the persilylated TMS ethers of cis/trans-isomers of tetrahydrodaidzein, were characterized based on the elucidation of fragments assocd. with the loss of a nonphenolic-OTMS functional group in ring-C. These are fragments presented in the persilylated mass spectra of isoflavan-4-ols and isoflav-3-ene-4-ols, demonstrated here by a combination of simple and tandem mass spectrometry study of the deuterated persilylated TMS ethers of dihydrodaidzein. In a similar study the authors also present the data on the structural identification and fragment elucidation of the keto/enol tautomers of the TMS ether derivs. of the dihydro derivs. of daidzein and genistein, obsd. in the urine of volunteers and considered probable products of the derivatization process. Finally, the GC and GC-MS data of two unknown isoflavonoids and that of a lignan-like compd. are presented together with those of dihydrodaidzein, dihydrogenistein, tetrahydrodaidzein and 2-dehydro-O-demethylangolensin. The latter four were obtained here as products of small scale chem. synthesis in a preliminary study on the tentative identification of urinary isoflavonoids in human volunteers challenged with soya.

IT 446-72-0, Genistein 486-66-8, Daidzein

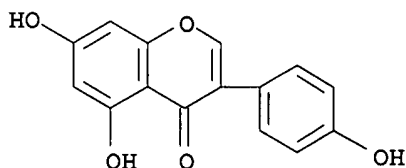
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PROC (Process)

(metabolic fate of human dietary **isoflavones** and  
**hydrogenation** of)

RN 446-72-0 CAPLUS

CN 4H-1-Benzopyran-4-one, 5,7-dihydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



RN 486-66-8 CAPLUS

CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)

